

Inosine
58-63-9 | DTXSID2045993

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.51

Global applicability domain: Inside

Local applicability domain index: 5.31e-01

Confidence level: 6.43e-01

Nearest Neighbors from the Training Set

Image not found

Inosine

Measured: -2.10

Predicted: -1.51

Image not found

N-[1,3-dihydroxy-2-(hydroxymethyl)propan-2-yl]-2-(2-nitroimidazol-1-yl)acetamide

Measured: -1.77

Predicted: -1.83

Image not found

Adenosine

Measured: -1.05

Predicted: -1.46

Image not found

2-Fluoroadenosine

Measured: -0.800

Predicted: -1.11